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Cooperative intramolecular hydrogen bond and conformations of thiocalix[4]arene molecules

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Abstract

The joint FTIR spectroscopic study and ab initio quantum-chemical calculations (HF/3-21G and PBE/TZ2P methods) showed that thiocalix[4] arene molecules adopt the cone conformation in CCl4 solutions. The weakening of the cooperative intramolecular H bond in thiocalix[4]arenes compared to the corresponding calix[4]arenes can be due to the larger thiocalixarene macrocycle, bifurcated hydrogen bond in it, and electron density transfer from the bridging S atom to the benzene ring.

Keywords

ab initio quantum-chemical calculations, Bifurcated hydrogen bond, Calix[4]arenes, Cone conformation, Cooperative hydrogen bond, FTIR spectroscopy, Thiocalix[4]arenes, UV spectroscopy